

09770562

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(FILE 'HOME' ENTERED AT 11:04:01 ON 08 JUL 2004)

FILE 'REGISTRY' ENTERED AT 11:05:19 ON 08 JUL 2004

L1 1 S NICARDIPINE/CN

L2 1 S NIFEDIPINE/CN

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L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 21829-25-4 REGISTRY

CN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl) -
, dimethyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(o-nitrophenyl) -
, dimethyl ester (8CI)

OTHER NAMES:

CN 2,6-Dimethyl-3,5-dicarbomethoxy-4-(2-nitrophenyl)-1,4-dihydropyridine

CN 2,6-Dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylic acid
dimethyl ester

CN 4-(2-Nitrophenyl)-2,6-dimethyl-3,5-dicarbomethoxy-1,4-dihydropyridine

CN Adalat

CN Adalat 10

CN Adalat 20

CN Adalat 5

CN Adalat CC

CN Adalat CR

CN Adalat Crono

CN Adalat FT

CN Adalat GITS

CN Adalat GITS 30

CN Adalat LA

CN Adalat LP

CN Adalat Oros

CN Adalat PA

CN Adalat Retard

CN Adalate

CN Adapine

CN Adapress

CN Alat

CN Aldipin

CN Alfadat

CN Alonix

CN Alonix S

CN Alpha-Nifedipine Retard

CN Angipec

CN Anifed

CN Anpine

CN Apo-Nifed

CN Aprical

CN BAY 1040

CN BAY-a 1040

CN Bonacid

CN Calcibloc

CN Calcigard

CN Calcilat

CN Camont

CN Cardifen

CN Cardilat

CN Cardilate

CN Cardionorm

CN Chronadalate

CN Chronadalate LP

CN Citilat

CN Coracten

CN Coral

CN Cordafen

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H donors (HD)	1		(1) ACD
Koc (KOC)	2.13	pH 1	(1) ACD
Koc (KOC)	587	pH 4	(1) ACD
Koc (KOC)	1090	pH 7	(1) ACD
Koc (KOC)	1091	pH 8	(1) ACD
Koc (KOC)	1091	pH 10	(1) ACD
logD (LOGD)	0.34	pH 1	(1) ACD
logD (LOGD)	2.78	pH 4	(1) ACD
logD (LOGD)	3.05	pH 7	(1) ACD
logD (LOGD)	3.05	pH 8	(1) ACD
logD (LOGD)	3.05	pH 10	(1) ACD
logP (LOGP)	3.054+/-0.590		(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	346.33		(1) ACD
pKa (PKA)	3.93+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	3.37E-09 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.67 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

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CN **Nifedipine**

ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for
DISPLAY

FS 3D CONCORD

DR 11104-22-6, 101539-70-2, 101554-38-5

MF C17 H18 N2 O6

CI COM

LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*,
BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CBNB,
CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSChem, CSNB, DDFU,
DETherm*, DIOGENES, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDb, IMSCoSEARCH,
IMSPATENTS, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PHAR, PROMT,
PROUSDDR, PS, RTECS*, SPECINFO, TOXCENTER, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, WHO

(**Enter CHEMLIST File for up-to-date regulatory information)

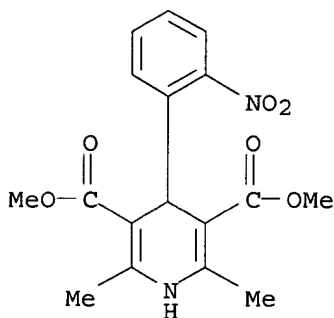
DT.CA Caplus document type: Book; Conference; Dissertation; Journal; Patent;
Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);
PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or
reagent); USES (Uses)

RLD.P Roles for non-specific derivatives from patents: ANST (Analytical
study); BIOL (Biological study); PREP (Preparation); PROC (Process);
USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological
study); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC
(Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical
study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP
(Preparation); PROC (Process); PRP (Properties); RACT (Reactant or
reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7031 REFERENCES IN FILE CA (1907 TO DATE)

102 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

7047 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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L2 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

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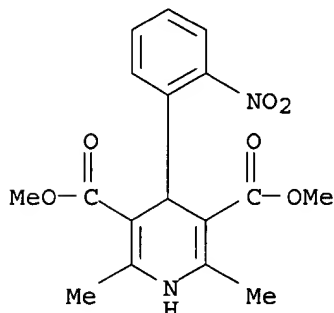
09770562

IN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl)-
, dimethyl ester (9CI)

ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT

MF C17 H18 N2 O6

CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d prop l2

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Melting Point (MP)	172-174 deg C		(1) IC
Melting Point (MP)	172-173 deg C	Solv: methanol (67-56-1)	(2) IC

(1) Cupka, Pavol; CS 243590 B1 1987 CAPLUS

(2) Loev, Bernard; Journal of Medicinal Chemistry 1974 V17(9) P956-65 CAPLUS

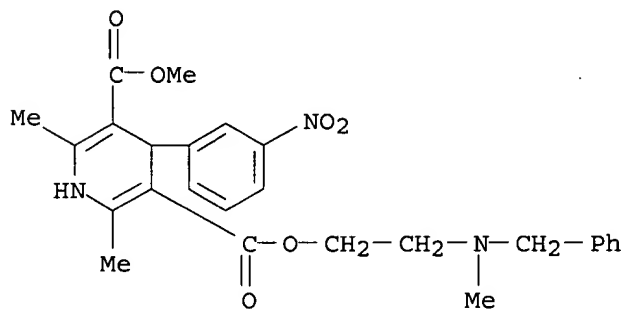
Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	66.3	pH 4	(1) ACD
Bioconc. Factor (BCF)	123	pH 7	(1) ACD
Bioconc. Factor (BCF)	123	pH 8	(1) ACD
Bioconc. Factor (BCF)	123	pH 10	(1) ACD
Boiling Point (BP)	475.3+/-45.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (Hvap)	73.87+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	241.2+/-51.7 deg C		(1) ACD
H acceptors (HAC)	8		(1) ACD

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L1 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-
, methyl 2-[methyl(phenylmethyl)amino]ethyl ester (9CI)
MF C26 H29 N3 O6
CI COM

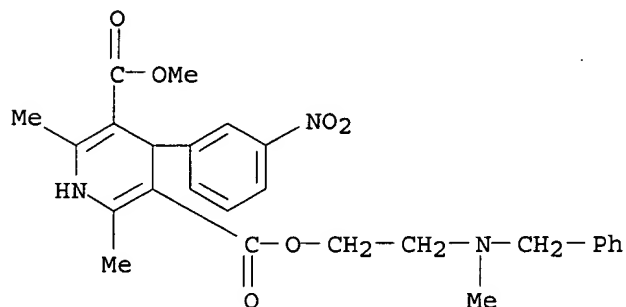


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L1 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-
methyl 2-[methyl(phenylmethyl)amino]ethyl ester (9CI)
MF C26 H29 N3 O6
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d prop

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Melting Point (MP)	168.5 deg C	Solv: acetone (67-64-1)	(1) IC

(1) Nakamoto, Yasumasa; JP 62059261 A2 1987 CAPLUS

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	5.04	pH 4	(1) ACD
Bioconc. Factor (BCF)	2395	pH 7	(1) ACD
Bioconc. Factor (BCF)	4841	pH 8	(1) ACD
Bioconc. Factor (BCF)	5454	pH 10	(1) ACD
Boiling Point (BP)	603.4+/-55.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	89.75+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	318.7+/-56.7 deg C		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD

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09770562

Koc (KOC)	15.2	pH 4	(1) ACD
Koc (KOC)	7220	pH 7	(1) ACD
Koc (KOC)	14592	pH 8	(1) ACD
Koc (KOC)	16440	pH 10	(1) ACD
logD (LOGD)	0.27	pH 1	(1) ACD
logD (LOGD)	2.19	pH 4	(1) ACD
logD (LOGD)	4.86	pH 7	(1) ACD
logD (LOGD)	5.17	pH 8	(1) ACD
logD (LOGD)	5.22	pH 10	(1) ACD
logP (LOGP)	5.221+/-0.622		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	479.53		(1) ACD
pKa (PKA)	7.11+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	1.63E-14 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.67 ((C) 1994-2004 ACD/Labs)

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